LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098803.D
Acq On : 26 Sep 2017 00:52
Operator : SJ/JU
Sample : I5391-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-015

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	21	25	35	rVB	91529	138881	3.13%	0.378%
2	5.151	516	521	533	rVB	515847	712304	16.06%	1.938%
3	5.540	581	587	590	rBV	3707604	3790013	85.45%	10.312%
4	6.540	750	757	760	rBV	3442648	3880202	87.48%	10.557%
5	6.687	776	782	785	rBV	3821861	3894130	87.79%	10.595%
6	6.910	817	820	824	rVB	1009138	897758	20.24%	2.443%
7	7.069	843	847	851	rBV	3241037	2966730	66.89%	8.072%
8	7.475	910	916	919	rBV	2416522	2452983	55.30%	6.674%
9	8.192	1034	1038	1042	rBV	1413059	1268131	28.59%	3.450%
10	9.269	1215	1221	1224	rBV	4285597	4435492	100.00%	12.068%
11	9.657	1283	1287	1290	rBV	433215	332791	7.50%	0.905%
12	9.951	1332	1337	1341	rVB	1610622	1411324	31.82%	3.840%
13	10.369	1405	1408	1411	rVB	69195	61703	1.39%	0.168%
14	10.739	1463	1471	1474	rBV	2341316	2247712	50.68%	6.116%
15	10.845	1486	1489	1495	rBV	94690	92918	2.09%	0.253%
16	11.439	1585	1590	1593	rBV	1504937	1371540	30.92%	3.732%
17	13.022	1854	1859	1862	rBV	3700166	3852038	86.85%	10.481%
18	13.904	2005	2009	2013	rBV	218287	214605	4.84%	0.584%
19	14.074	2034	2038	2042	rVB	1071558	930185	20.97%	2.531%
20	14.533	2113	2116	2120	rBV3	59276	68113	1.54%	0.185%
21	15.192	2224	2228	2235	rVB	135093	167349	3.77%	0.455%
22	15.563	2286	2291	2301	rVB	640827	875706	19.74%	2.383%
23	16.027	2365	2370	2375	rBV	131034	194143	4.38%	0.528%
24	16.551	2454	2459	2466	rVB2	71429	121121	2.73%	0.330%
25	17.162	2558	2563	2572	rVB2	64132	133700	3.01%	0.364%
26	17.662	2643	2648	2653	rBV8	49793	101617	2.29%	0.276%
27	18.509	2786	2792	2796	rBV7	37299	84998	1.92%	0.231%
28	18.739	2827	2831	2838	rVB9	23876	55958	1.26%	0.152%

Sum of corrected areas: 36754145

LSC Report - Integrated Chromatogram

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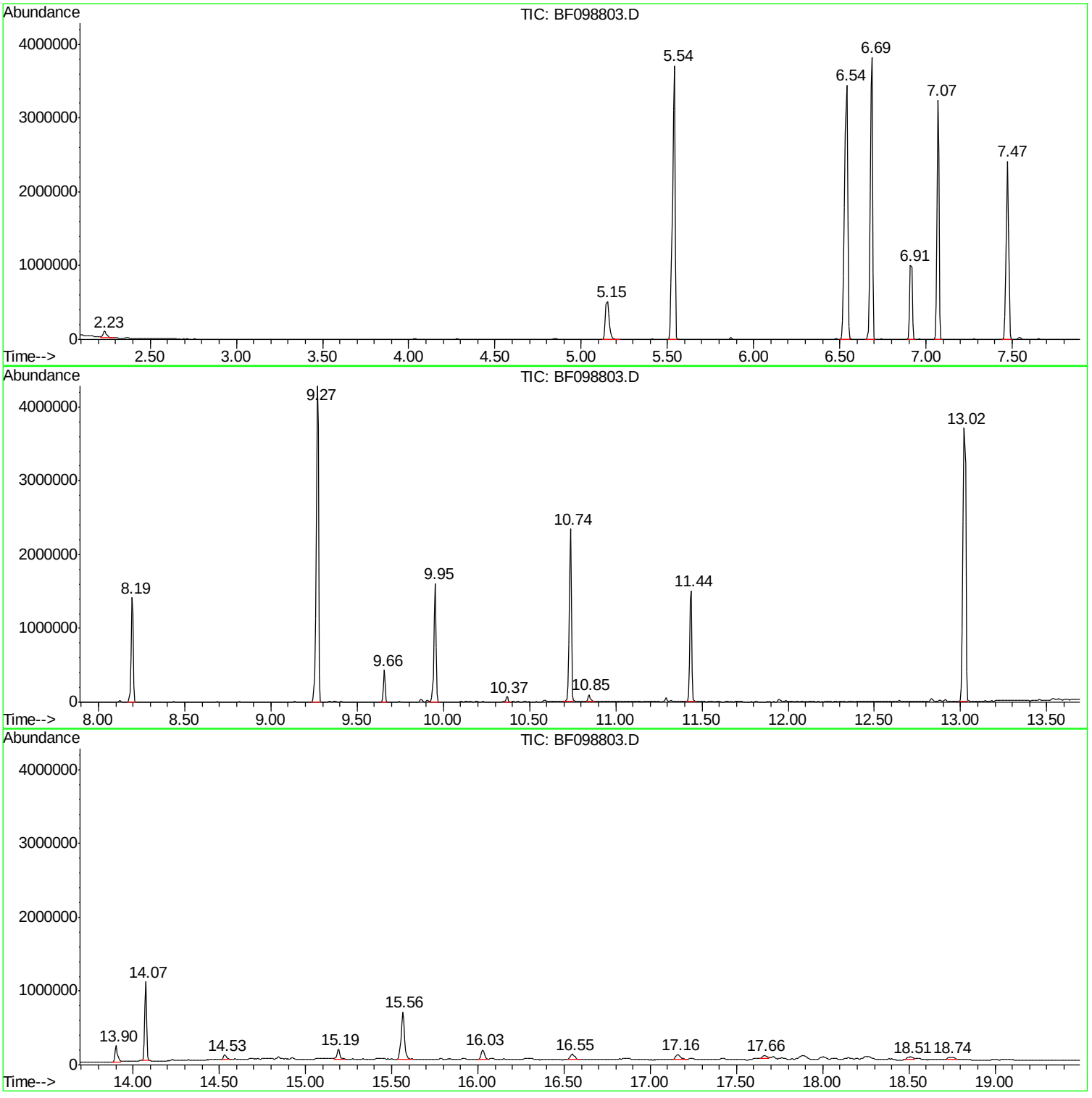
Operator : SJ/JU
Sample : I5391-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098803.D
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Operator : SJ/JU
Sample : I5391-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

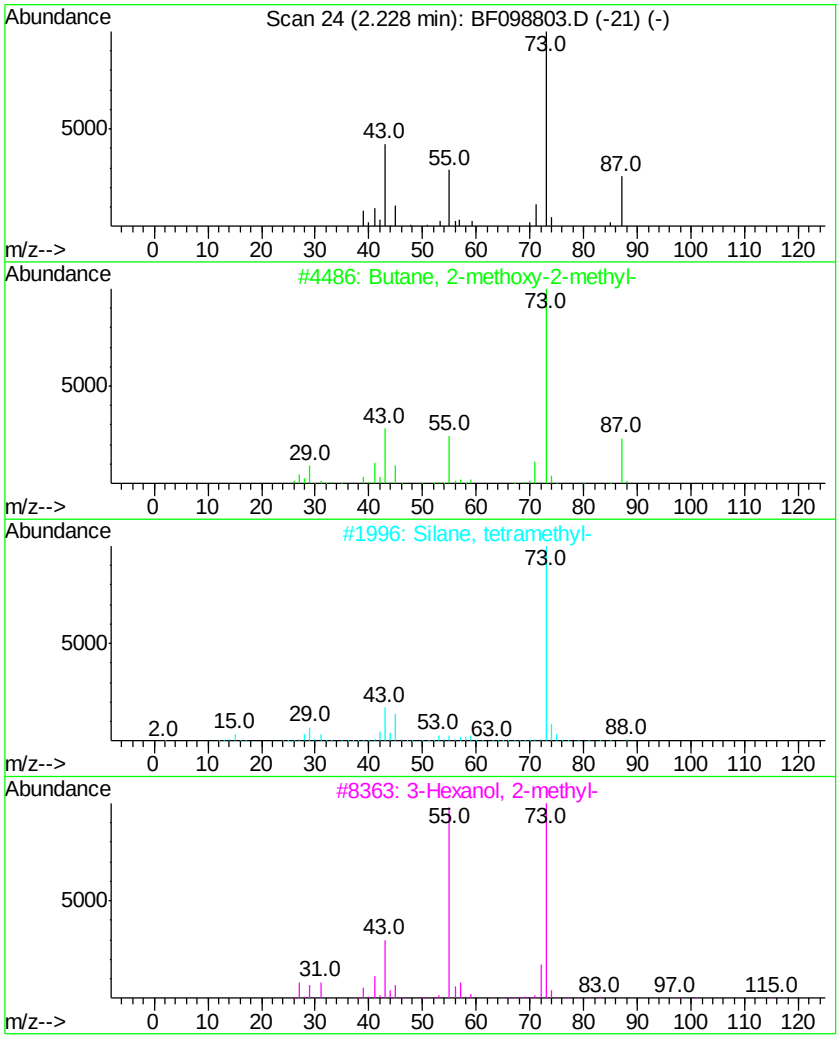
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

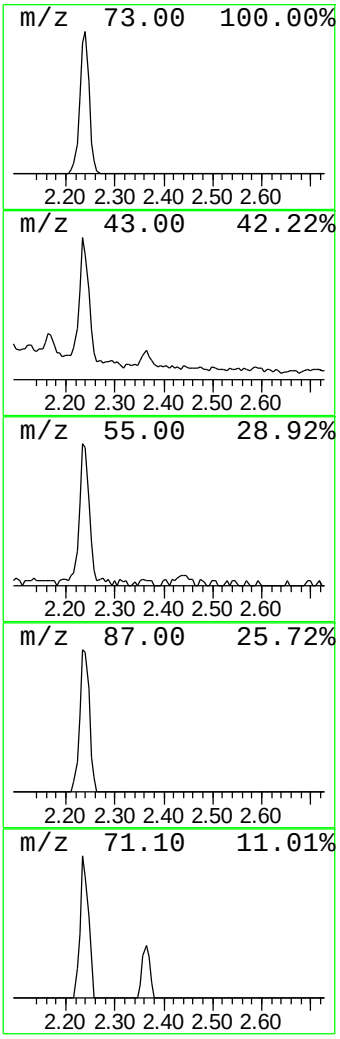
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	3.09 ng	138881	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098803.D
Acq On : 26 Sep 2017 00:52
Operator : SJ/JU
Sample : I5391-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

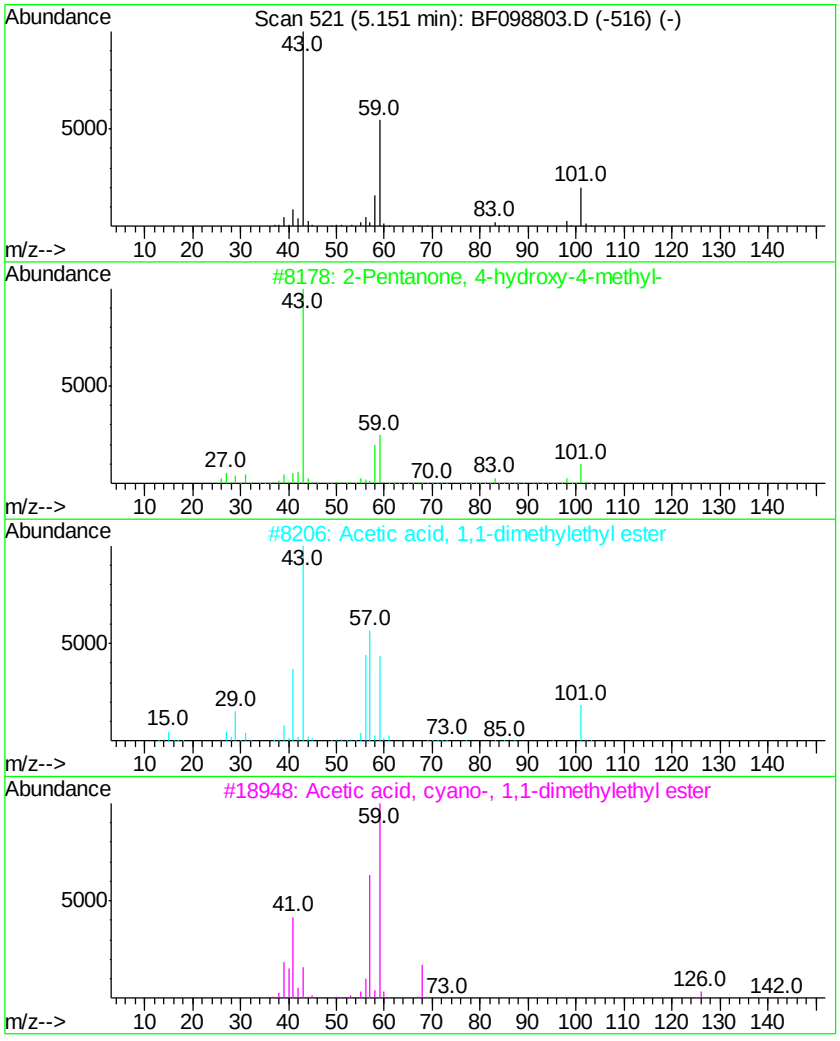
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

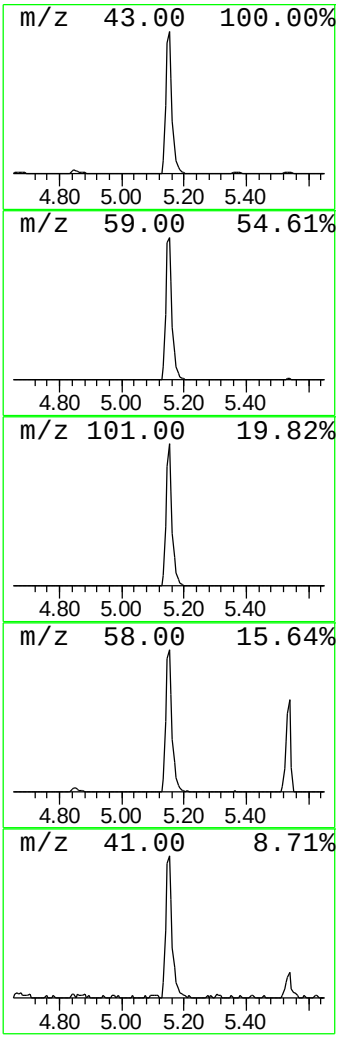
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	15.87 ng	712304	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098803.D
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Operator : SJ/JU
Sample : I5391-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

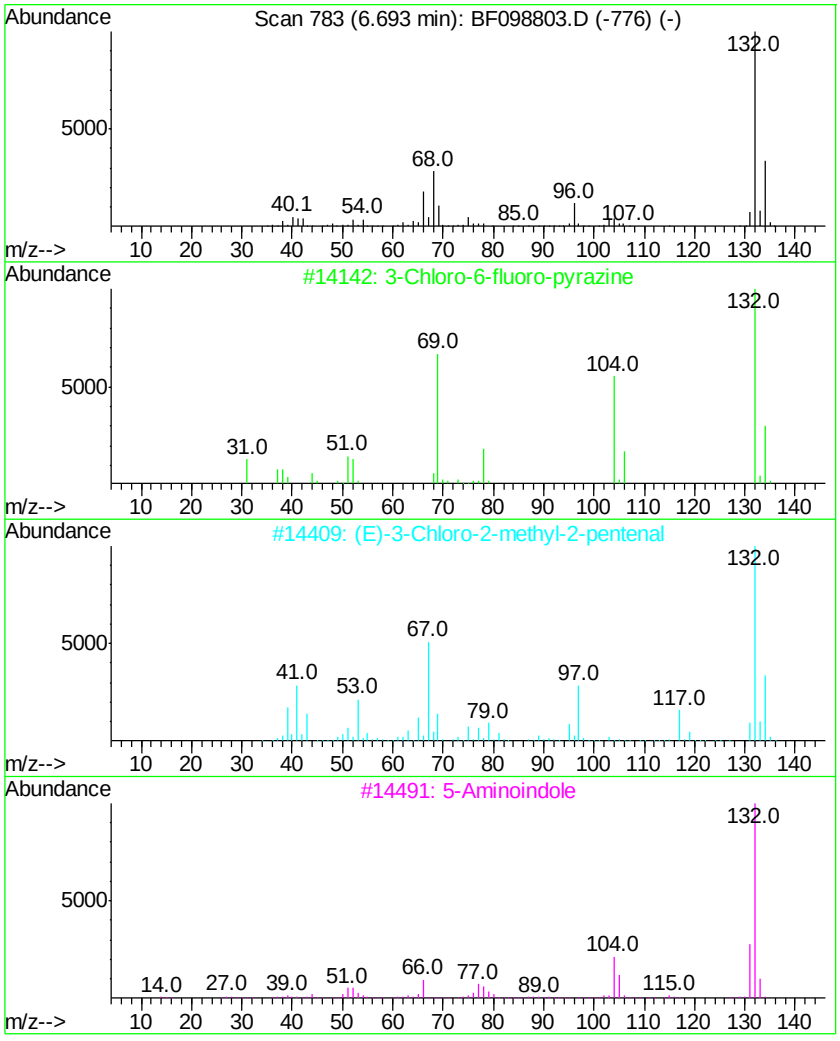
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

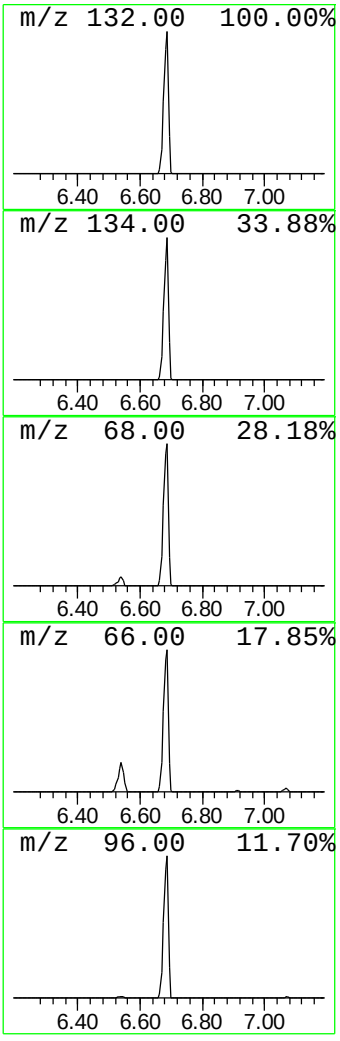
****

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	86.75 ng	3894130	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
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Operator : SJ/JU
Sample : I5391-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

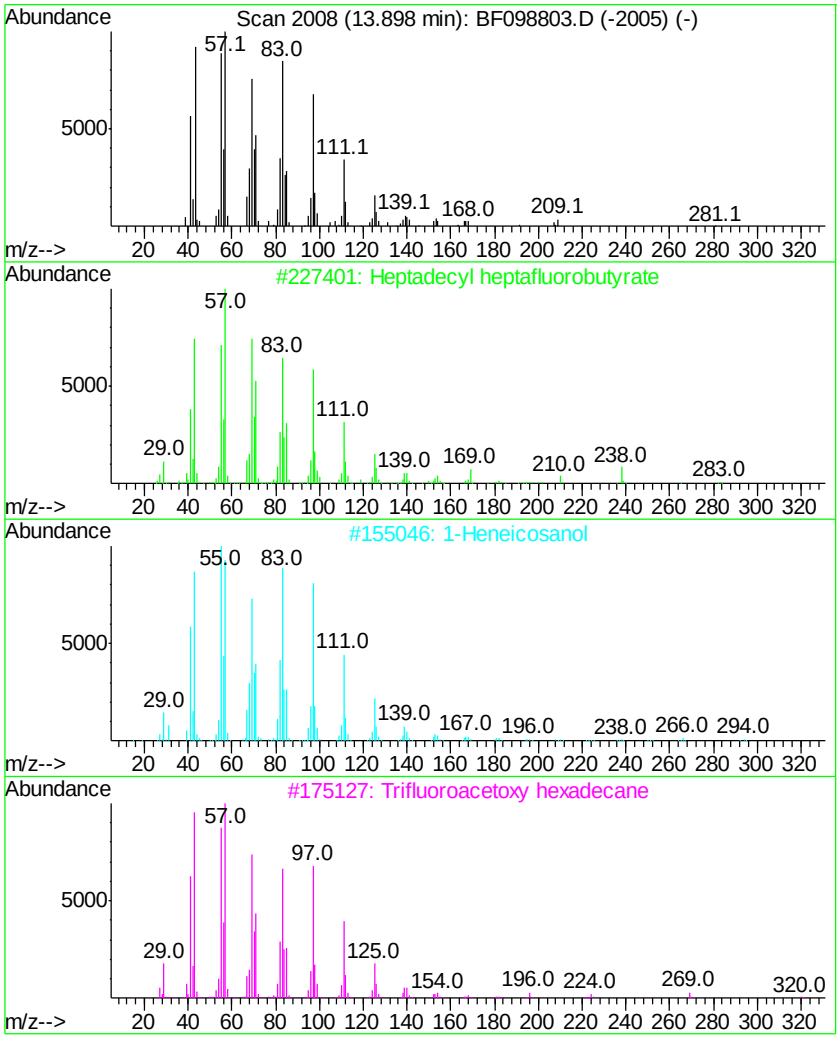
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

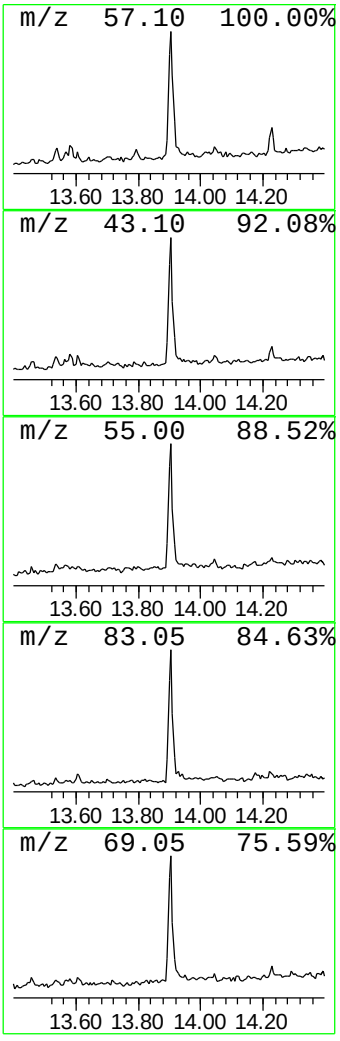
****

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	4.61 ng	214605	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	95





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098803.D
Acq On : 26 Sep 2017 00:52
Operator : SJ/JU
Sample : I5391-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

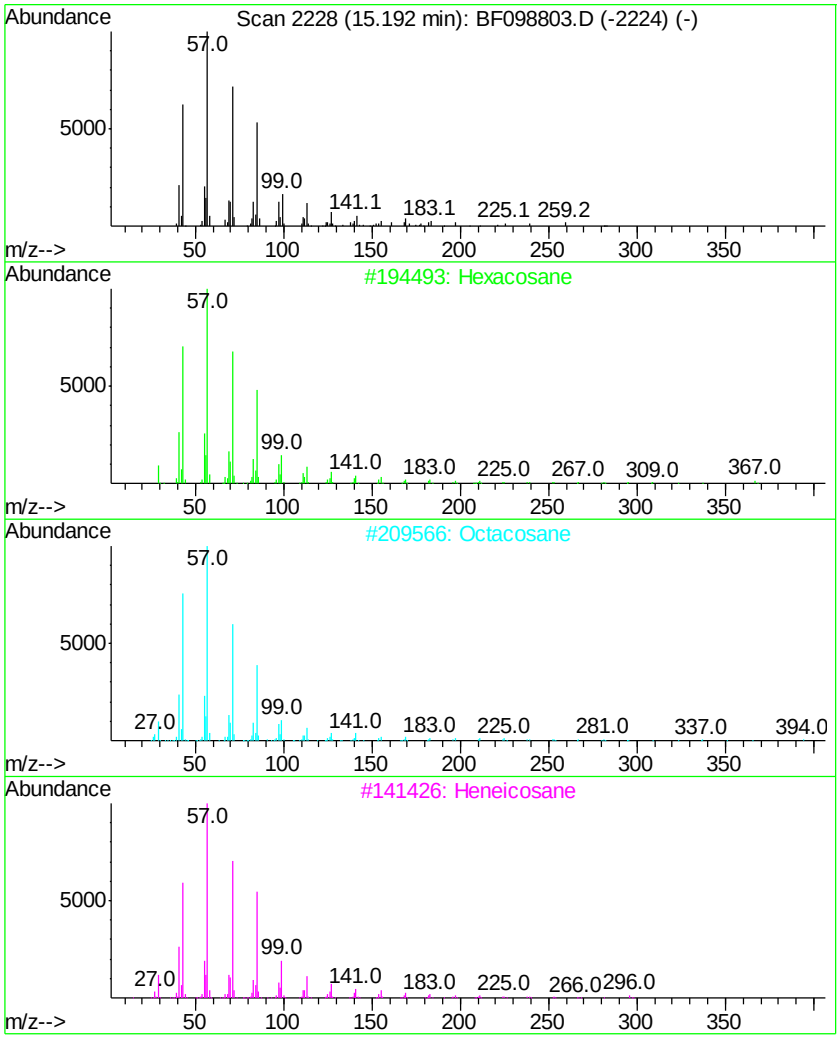
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

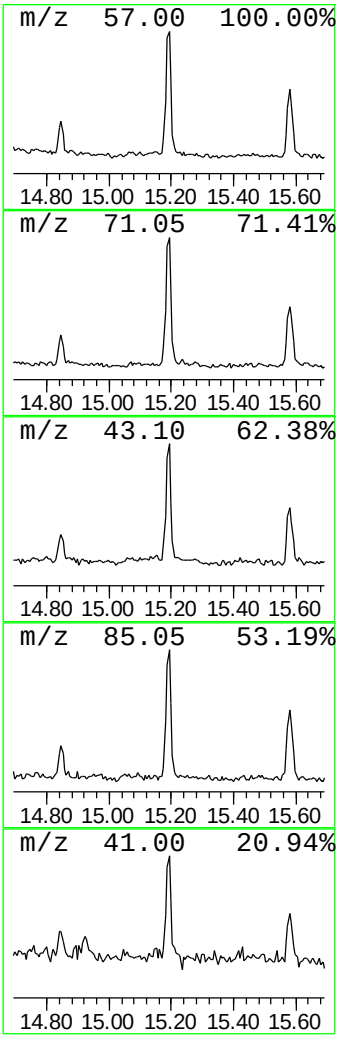
****

Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	3.82 ng	167349	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Octadecane	254	C18H38	000593-45-3	91





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Sample : I5391-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

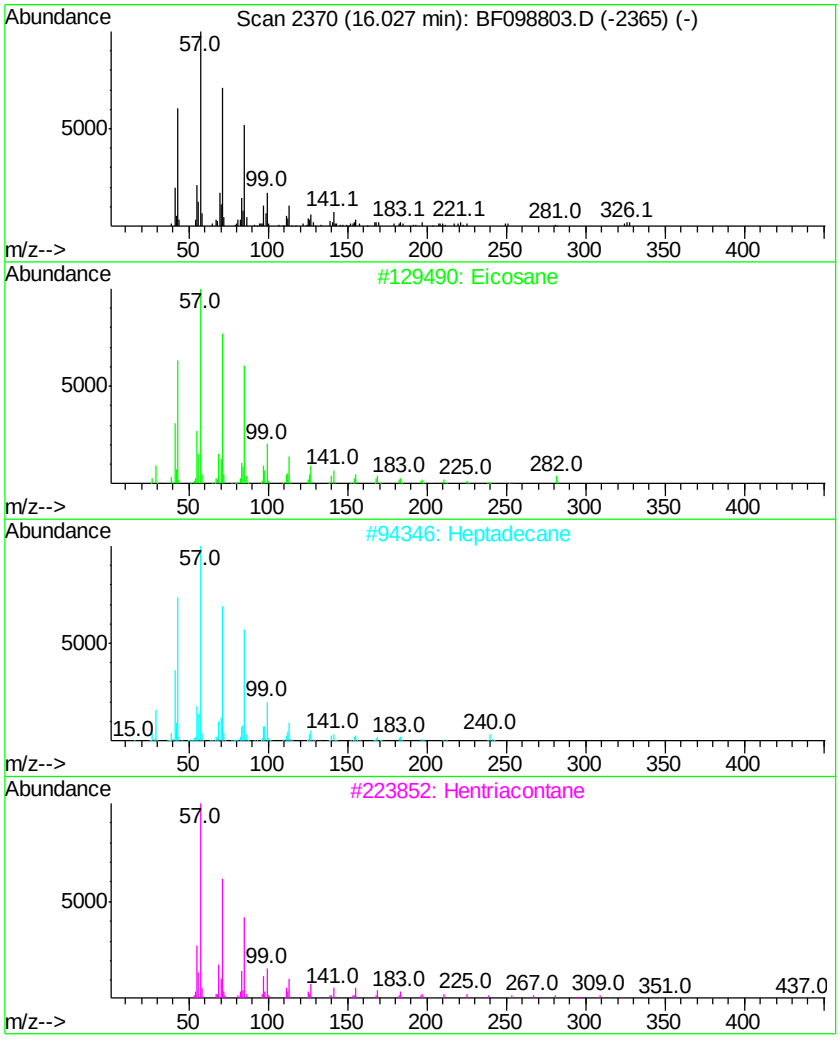
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

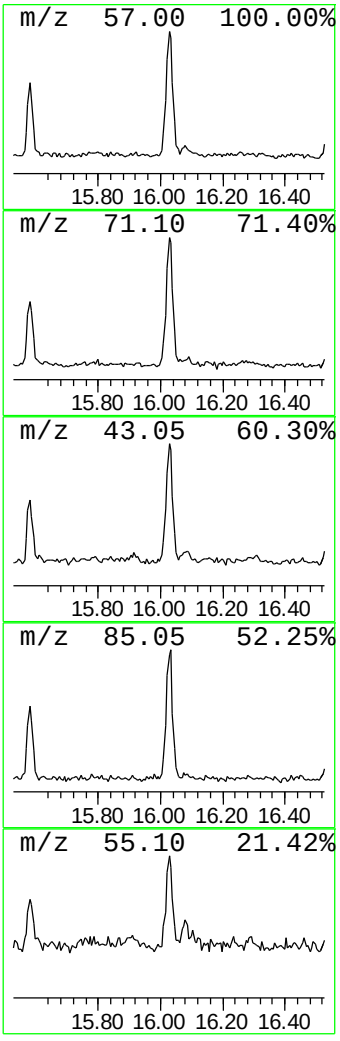
****

Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	4.43 ng	194143	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heptadecane	240	C17H36	000629-78-7	90
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Tetracosane	338	C24H50	000646-31-1	90





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Sample : I5391-01
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Instrument : BNA_F
ClientSampleId : FK-PS-01-015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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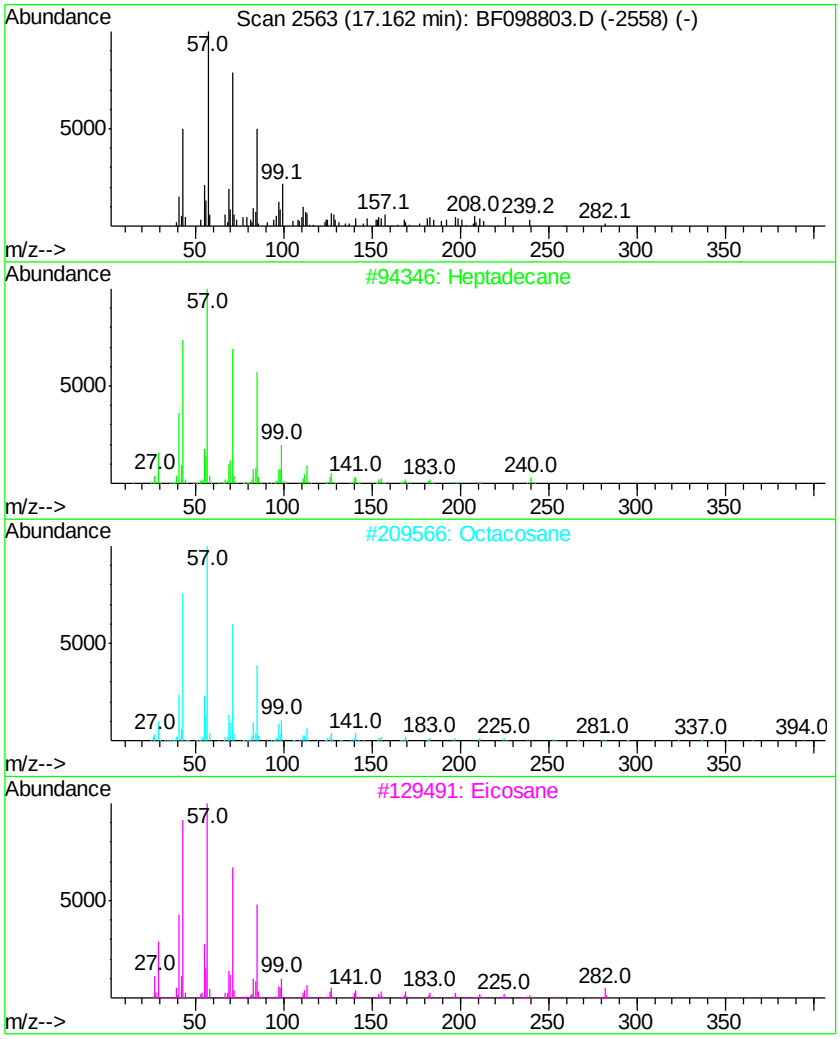
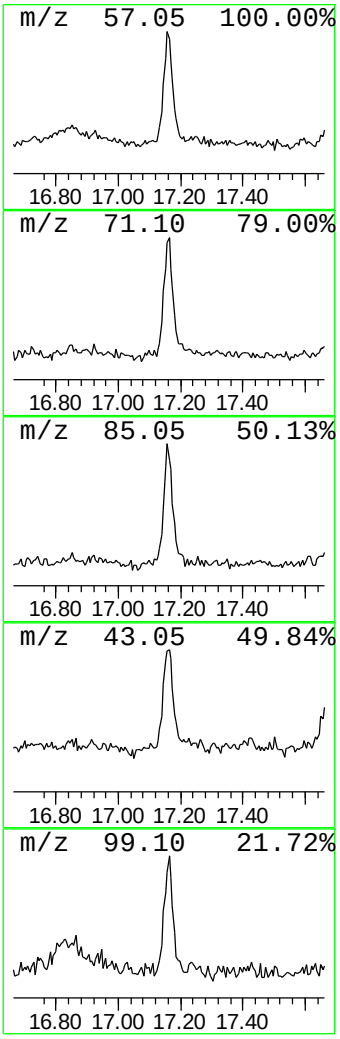
Peak Number 9 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	3.05 ng	133700	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	80
2	Octacosane	394	C28H58	000630-02-4	72
3	Eicosane	282	C20H42	000112-95-8	64
4	Nonadecane	268	C19H40	000629-92-5	64
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64





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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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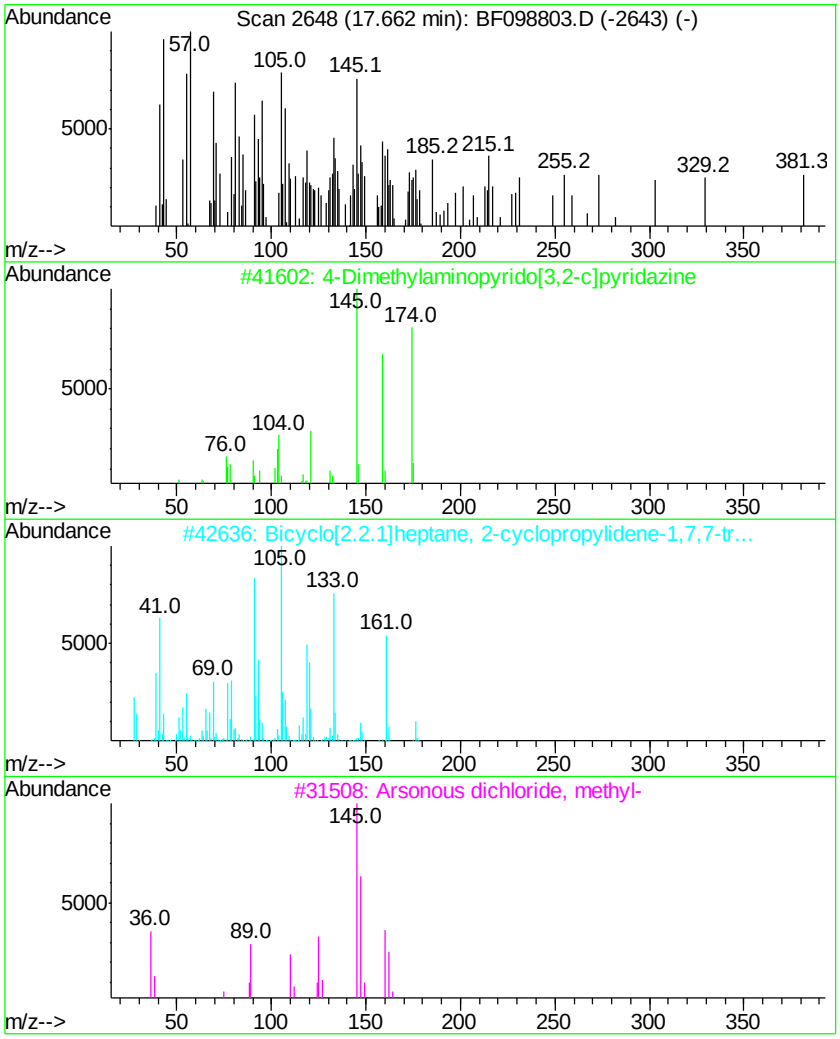
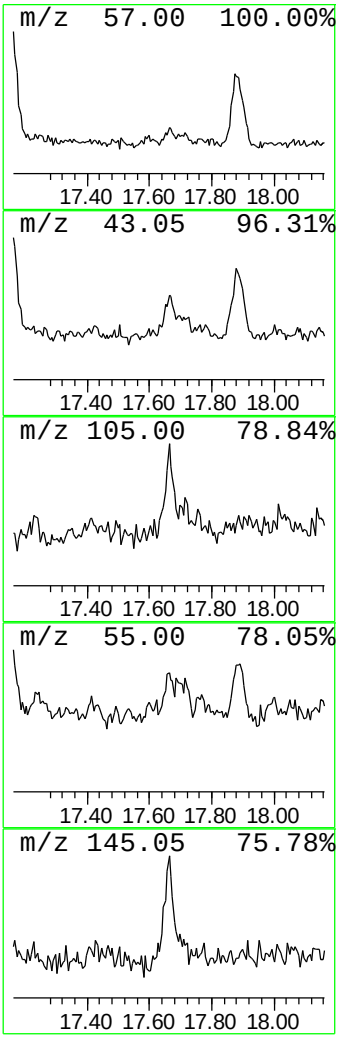
Peak Number 10 unknown17.66 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.66	2.32 ng	101617	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Dimethylaminopyrido[3,2-c]pyri...	174	C9H10N4	1000326-90-5	22
2	Bicyclo[2.2.1]heptane, 2-cyclopr...	176	C13H20	1000159-45-7	22
3	Arsonous dichloride, methyl-	160	CH3AsCl2	000593-89-5	18
4	Acrylonitrile, .beta.-[3-(2,2-di...	189	C13H19N	1000154-20-7	15
5	Megastigma-4,6(E),8(Z)-triene	176	C13H20	071186-24-8	14





Tentatively Identified Compound (LSC) summary

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Operator : SJ/JU
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.23	3.1	ng	138881	1	6.92	897758	20.0
2-Pentanone, 4-hy...	5.15	15.9	ng	712304	1	6.92	897758	20.0
unknown6.69	6.69	86.8	ng	3894130	1	6.92	897758	20.0
Heptadecyl heptaf...	13.90	4.6	ng	214605	5	14.07	930185	20.0
Hexacosane	15.19	3.8	ng	167349	6	15.56	875706	20.0
Eicosane	16.03	4.4	ng	194143	6	15.56	875706	20.0
Heptadecane	17.16	3.0	ng	133700	6	15.56	875706	20.0
unknown17.66	17.66	2.3	ng	101617	6	15.56	875706	20.0